



Full wwPDB X-ray Structure Validation Report ⓘ

May 21, 2020 – 03:29 pm BST

PDB ID : 2OEX
Title : Structure of ALIX/AIP1 V Domain
Authors : Fisher, R.D.; Zhai, Q.; Robinson, H.; Hill, C.P.
Deposited on : 2007-01-01
Resolution : 2.58 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

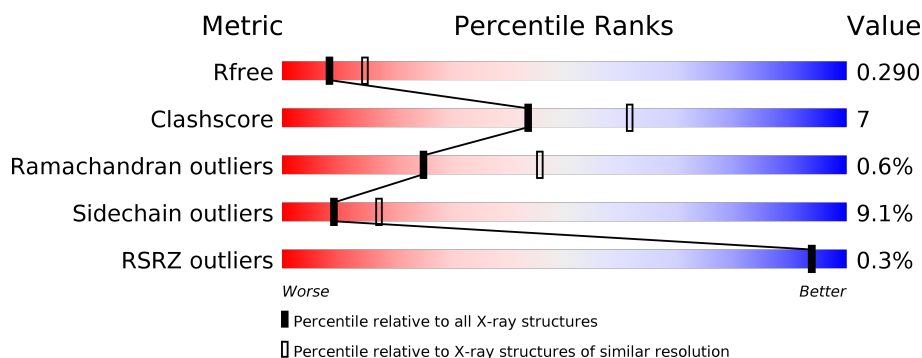
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.58 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3676 (2.60-2.56)
Clashscore	141614	4049 (2.60-2.56)
Ramachandran outliers	138981	3979 (2.60-2.56)
Sidechain outliers	138945	3979 (2.60-2.56)
RSRZ outliers	127900	3614 (2.60-2.56)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	351	
1	B	351	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5489 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Programmed cell death 6-interacting protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	342	Total	C	N	O	S	Se	0	0	0
			2699	1674	475	543	3	4			
1	B	341	Total	C	N	O	S	Se	0	1	0
			2701	1674	475	545	3	4			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	352	GLY	-	CLONING ARTIFACT	UNP Q8WUM4
A	353	ILE	-	CLONING ARTIFACT	UNP Q8WUM4
A	354	ASP	-	CLONING ARTIFACT	UNP Q8WUM4
A	355	PRO	-	CLONING ARTIFACT	UNP Q8WUM4
A	356	PHE	-	CLONING ARTIFACT	UNP Q8WUM4
A	357	THR	-	CLONING ARTIFACT	UNP Q8WUM4
A	358	HIS	-	CLONING ARTIFACT	UNP Q8WUM4
A	359	MET	-	CLONING ARTIFACT	UNP Q8WUM4
A	385	MSE	MET	MODIFIED RESIDUE	UNP Q8WUM4
A	543	MSE	MET	MODIFIED RESIDUE	UNP Q8WUM4
A	580	MSE	MET	MODIFIED RESIDUE	UNP Q8WUM4
A	639	MSE	MET	MODIFIED RESIDUE	UNP Q8WUM4
B	352	GLY	-	CLONING ARTIFACT	UNP Q8WUM4
B	353	ILE	-	CLONING ARTIFACT	UNP Q8WUM4
B	354	ASP	-	CLONING ARTIFACT	UNP Q8WUM4
B	355	PRO	-	CLONING ARTIFACT	UNP Q8WUM4
B	356	PHE	-	CLONING ARTIFACT	UNP Q8WUM4
B	357	THR	-	CLONING ARTIFACT	UNP Q8WUM4
B	358	HIS	-	CLONING ARTIFACT	UNP Q8WUM4
B	359	MET	-	CLONING ARTIFACT	UNP Q8WUM4
B	385	MSE	MET	MODIFIED RESIDUE	UNP Q8WUM4
B	543	MSE	MET	MODIFIED RESIDUE	UNP Q8WUM4
B	580	MSE	MET	MODIFIED RESIDUE	UNP Q8WUM4
B	639	MSE	MET	MODIFIED RESIDUE	UNP Q8WUM4

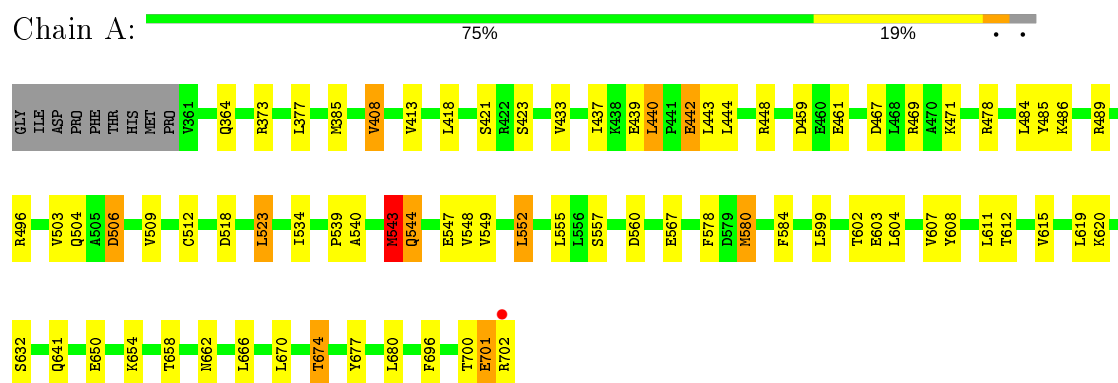
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	47	Total 47	O 47	0	0
2	B	42	Total 42	O 42	0	0

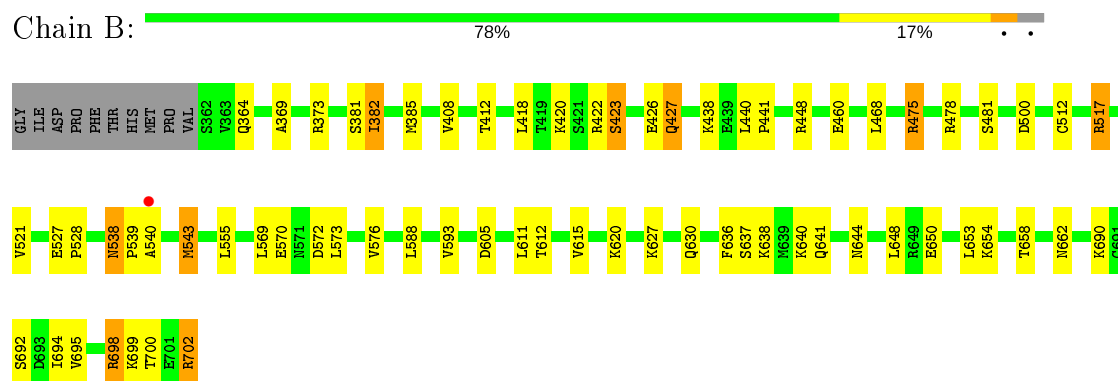
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Programmed cell death 6-interacting protein



- Molecule 1: Programmed cell death 6-interacting protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	63.86Å 50.05Å 130.17Å 90.00° 101.13° 90.00°	Depositor
Resolution (Å)	50.00 – 2.58 40.95 – 2.58	Depositor EDS
% Data completeness (in resolution range)	91.0 (50.00-2.58) 91.5 (40.95-2.58)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.63 (at 2.58Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.228 , 0.302 0.220 , 0.290	Depositor DCC
R_{free} test set	1142 reflections (4.81%)	wwPDB-VP
Wilson B-factor (Å ²)	39.8	Xtriage
Anisotropy	0.661	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 26.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	5489	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.57% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.54	0/2722	0.63	0/3665
1	B	0.52	0/2724	0.64	1/3667 (0.0%)
All	All	0.53	0/5446	0.64	1/7332 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	468	LEU	CA-CB-CG	5.29	127.46	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2699	0	2734	42	0
1	B	2701	0	2730	31	0
2	A	47	0	0	4	0
2	B	42	0	0	2	0
All	All	5489	0	5464	73	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (73) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:701:GLU:HG3	1:A:702:ARG:H	1.25	1.02
1:A:662:ASN:O	1:A:666:LEU:HG	1.67	0.94
1:A:385:MSE:HE3	1:A:615:VAL:HG22	1.55	0.89
1:A:578:PHE:CE2	1:A:580:MSE:HE3	2.20	0.77
1:A:578:PHE:HE2	1:A:580:MSE:HE3	1.50	0.75
1:A:580:MSE:HE1	1:A:603:GLU:HG3	1.69	0.74
1:A:444:LEU:HD11	1:A:503:VAL:HG22	1.69	0.74
1:A:543:MSE:HG3	1:A:549:VAL:HG21	1.69	0.74
1:A:385:MSE:CE	1:A:615:VAL:HG22	2.23	0.68
1:A:701:GLU:HG3	1:A:702:ARG:N	2.04	0.67
1:A:578:PHE:HE2	1:A:580:MSE:CE	2.07	0.66
1:B:448:ARG:NH2	1:B:500:ASP:OD1	2.24	0.66
1:B:475:ARG:HH11	1:B:475:ARG:HG2	1.60	0.65
1:B:540:ALA:HB1	1:B:543:MSE:HG2	1.79	0.65
1:A:580:MSE:CE	1:A:580:MSE:HA	2.27	0.65
1:B:385:MSE:HE2	1:B:385:MSE:HA	1.78	0.64
1:A:459:ASP:OD1	1:A:489:ARG:NH2	2.31	0.63
1:B:650:GLU:O	1:B:654:LYS:HG3	2.01	0.60
1:A:650:GLU:HG2	1:A:654:LYS:HE2	1.85	0.59
1:A:580:MSE:HA	1:A:580:MSE:HE2	1.85	0.59
1:B:517:ARG:O	1:B:521:VAL:HG23	2.03	0.58
1:B:644:ASN:O	1:B:648:LEU:HG	2.02	0.58
1:B:527:GLU:HB3	1:B:528:PRO:HD3	1.85	0.58
1:B:478:ARG:HD3	1:B:702:ARG:HD3	1.86	0.57
1:A:602:THR:HG23	2:A:28:HOH:O	2.05	0.56
1:B:690:LYS:O	1:B:694:ILE:HG12	2.06	0.56
1:A:603:GLU:O	1:A:607:VAL:HG22	2.06	0.55
1:A:696:PHE:O	1:A:700:THR:HB	2.07	0.55
1:A:461:GLU:HG2	1:A:485:TYR:OH	2.06	0.55
1:A:413:VAL:HG21	1:A:418:LEU:HD13	1.90	0.55
1:A:444:LEU:HG	1:A:677:TYR:OH	2.06	0.54
1:B:475:ARG:NH1	1:B:475:ARG:HG2	2.23	0.54
1:A:439:GLU:HA	1:A:442:GLU:HG3	1.90	0.53
1:A:440:LEU:HD21	1:A:674:THR:HG22	1.89	0.53
1:B:481:SER:OG	1:B:698:ARG:NH1	2.42	0.53
1:A:670:LEU:O	1:A:674:THR:HG23	2.09	0.52
1:B:381:SER:HB3	1:B:573:LEU:HD21	1.91	0.52
1:A:578:PHE:CE2	1:A:580:MSE:CE	2.89	0.51
1:A:448:ARG:NH1	2:A:39:HOH:O	2.43	0.51
1:A:408:VAL:O	1:A:539:PRO:HB3	2.12	0.50
1:A:478:ARG:HH12	1:A:702:ARG:CZ	2.24	0.50
1:B:460:GLU:HB3	2:B:22:HOH:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:467:ASP:OD1	1:A:471:LYS:HE3	2.12	0.49
1:A:437:ILE:CD1	1:A:670:LEU:HD21	2.44	0.48
1:B:538:ASN:HB2	1:B:641:GLN:HE21	1.79	0.48
1:A:373:ARG:HB3	1:A:604:LEU:HD11	1.96	0.47
1:A:658:THR:O	1:A:662:ASN:ND2	2.47	0.47
1:B:423:SER:O	1:B:427:GLN:HB2	2.15	0.47
1:A:506:ASP:O	1:A:509:VAL:HG12	2.14	0.47
1:A:469:ARG:HD3	2:A:26:HOH:O	2.14	0.47
1:B:611:LEU:O	1:B:615:VAL:HG23	2.15	0.47
1:B:440:LEU:N	1:B:441:PRO:HD2	2.31	0.46
1:A:421:SER:HA	1:A:523:LEU:HD22	1.98	0.45
1:B:695:VAL:O	1:B:699:LYS:HG3	2.16	0.45
1:B:408:VAL:O	1:B:539:PRO:HA	2.17	0.44
1:B:658:THR:HG22	1:B:662:ASN:OD1	2.18	0.44
1:A:377:LEU:HD23	1:A:377:LEU:C	2.39	0.43
1:B:572:ASP:O	1:B:576:VAL:HG23	2.18	0.43
1:B:637:SER:HA	1:B:640:LYS:HE3	2.00	0.43
1:A:543:MSE:HG2	1:A:544:GLN:N	2.34	0.43
1:B:369:ALA:HB1	1:B:373:ARG:NH2	2.34	0.42
1:A:552:LEU:HD13	1:A:632:SER:HB2	2.01	0.42
1:B:478:ARG:HH11	1:B:702:ARG:HD2	1.85	0.42
1:B:382:ILE:HG12	1:B:570:GLU:HG3	2.01	0.42
1:B:381:SER:CB	1:B:573:LEU:HD21	2.50	0.41
1:B:418:LEU:HG	1:B:422:ARG:NH1	2.36	0.41
1:B:636:PHE:C	1:B:638:LYS:H	2.23	0.41
1:A:608:TYR:O	1:A:612:THR:HG23	2.21	0.41
1:A:701:GLU:CG	1:A:702:ARG:H	2.09	0.41
1:B:569:LEU:O	1:B:573:LEU:HB2	2.21	0.41
1:A:504:GLN:HB3	2:A:80:HOH:O	2.21	0.40
1:A:540:ALA:HA	1:A:641:GLN:HE21	1.86	0.40
1:B:420:LYS:HE2	2:B:5:HOH:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	340/351 (97%)	329 (97%)	8 (2%)	3 (1%)	17	34
1	B	340/351 (97%)	323 (95%)	16 (5%)	1 (0%)	41	62
All	All	680/702 (97%)	652 (96%)	24 (4%)	4 (1%)	25	45

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	544	GLN
1	B	538	ASN
1	A	543	MSE
1	A	701	GLU

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	303/307 (99%)	272 (90%)	31 (10%)	7	13
1	B	303/307 (99%)	279 (92%)	24 (8%)	12	23
All	All	606/614 (99%)	551 (91%)	55 (9%)	9	17

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	364	GLN
1	A	408	VAL
1	A	423	SER
1	A	433	VAL
1	A	440	LEU
1	A	442	GLU
1	A	443	LEU
1	A	484	LEU
1	A	486	LYS

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Mol	Chain	Res	Type
1	A	496	ARG
1	A	506	ASP
1	A	512	CYS
1	A	518	ASP
1	A	523	LEU
1	A	534	ILE
1	A	543	MSE
1	A	547	GLU
1	A	548	VAL
1	A	552	LEU
1	A	555	LEU
1	A	557	SER
1	A	560	ASP
1	A	567	GLU
1	A	580	MSE
1	A	584	PHE
1	A	599	LEU
1	A	611	LEU
1	A	619	LEU
1	A	620	LYS
1	A	674	THR
1	A	680	LEU
1	B	364	GLN
1	B	382	ILE
1	B	412	THR
1	B	423	SER
1	B	426	GLU
1	B	427	GLN
1	B	438	LYS
1	B	475	ARG
1	B	512	CYS
1	B	517	ARG
1	B	543	MSE
1	B	555	LEU
1	B	588	LEU
1	B	593	VAL
1	B	605	ASP
1	B	612	THR
1	B	620	LYS
1	B	627	LYS
1	B	630	GLN
1	B	653	LEU

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Mol	Chain	Res	Type
1	B	692	SER
1	B	698	ARG
1	B	700	THR
1	B	702	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	641	GLN
1	A	644	ASN
1	B	531	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	338/351 (96%)	-0.17	1 (0%) 94 94	27, 46, 64, 85	0
1	B	337/351 (96%)	-0.13	1 (0%) 94 94	27, 48, 74, 104	0
All	All	675/702 (96%)	-0.15	2 (0%) 94 94	27, 47, 68, 104	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	702	ARG	2.2
1	B	540	ALA	2.1

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.